NERSC: HPC for Discovery and Innovation

The Department of Energy's Office of Science has, for 40 years, sent its biggest challenges in computer simulation and data analysis to a supercomputing center in California. The National Energy Research Scientific Computing (NERSC) facility is where over 6,000 DOE researchers find reliable and advanced high performance computing (HPC) solutions. The computational engine behind DOE's discovery science is now available to energy innovators in the private sector. Enhancing the nation's economic competitiveness through greater access to HPC capabilities is a strategic theme of the National Strategic Computing Initiative, announced in July 2015. NERSC welcomes partnerships in HPC to achieve those goals as exascale machines take shape.

In 2015, NERSC partnered with 130 industry users from 50 companies. The following pages highlight some of this work with private-sector researchers in renewable energy technologies, advanced manufacturing and energy resource modeling. New opportunities for HPC-driven collaborations are emerging in 2016.

If accelerating your innovation requires advanced computing, ask NERSC about HPC. To learn how NERSC can become part of your innovation agenda, see the back page of this brochure.

BERKELEY LAB

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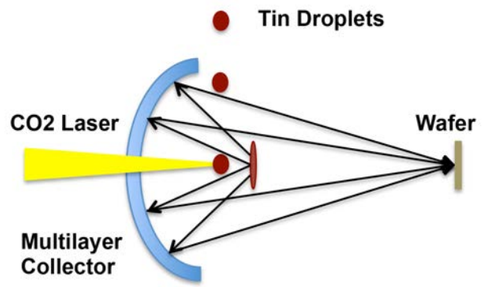
High Performance Computing (HPC) is part of the solution in deploying energy efficient technologies and advancing renewable energy sources. NERSC has long been known for the productivity of our users and a user-driven approach to HPC systems. In 2015 NERSC users turned 2 billion hours of computing time into over 1900 peer-reviewed publications. In the examples below the same HPC that powers scientific discovery is applied to energy innovation.

Deploying Renewables

Supercomputers have made their mark on climate simulation as a powerful tool for understanding future energy scenarios. The renewable energy from wind is directly tied to the same simulations and Vertum Partners has a Small Business Innovative Research (SBIR) Grant that provides the HPC to power future wind models to inform turbine placement. (http://www.vertumpartners.com/phone/apr2015a.html, presented at 15th Annual WRF Users Conference)

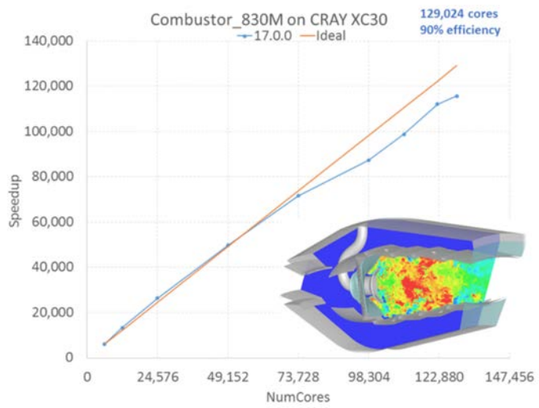
Advanced Manufacturing

Photolithography enables the miniaturizing of digital devices, allowing small (< 22nm) integrated circuitry to be masked onto chip substrates. Cymer Inc. is leveraging advanced AMR (adaptive mesh refinement) codes developed by DOE to simulate EUV photolithography for next-generation integrated circuits. Detailed simulations include the entire laser/metal/wafer system to allow simulation of processes which are too resource-intensive for experimental approaches.



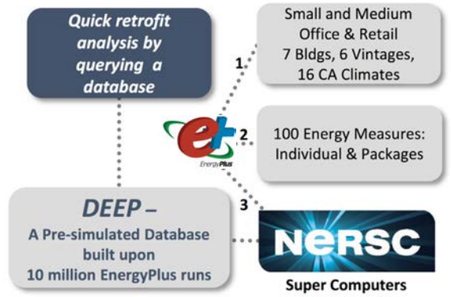
Scalable Simulation

HPC brings speed through scale. ANSYS and Cray Inc., working in conjunction with NERSC, have smashed the previous simulation world record by scaling the commercial Fluent code to 129,000 compute cores—enabling organizations to spur innovation by creating complete virtual prototypes of their products. Running simulations 100,000 times faster with HPC is not just faster, it's a wholly different capability.



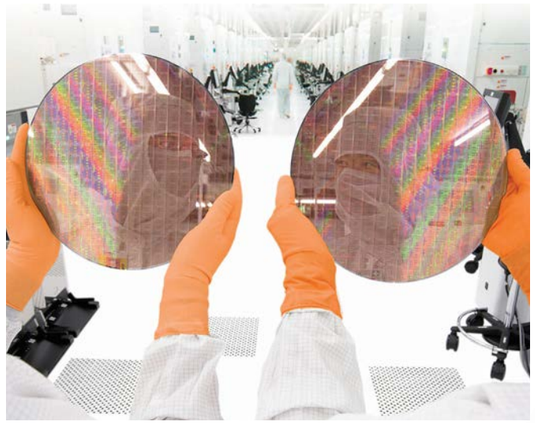
Energy Efficient Buildings

Database of Energy Efficiency Performance (DEEP) enables a quick retrofit analysis for small and medium sized office and retail buildings in California by querying a database built upon about 10 million EnergyPlus simulations run on DOE's NERSC center. DEEP powers the preliminary retrofit analysis of the Commercial Building Energy Saver (CBES) Toolkit.



Ultra-low Power Chips

The points of contact between metal wires and semiconductors are a key source of thermal waste in electronic devices. GlobalFoundries is pushing boundaries in atomistic simulation of device components by studying how energy is lost where wires meet chips. The findings of this work are being used to guide the GLOBALFOUNDRIES's 22nm FDSOI chip. Ultra-low power nano-electronics can be studied using the same HPC codes developed by DOE researchers in materials science. Advances in energy efficient digital devices advance multiple DOE program agendas.



Better Batteries

HPC is one of the tools in innovating how batteries store and deliver energy. Quatumscape Inc. studies novel battery designs using community materials science codes. These simulations help validate reactive MD forcefields which are used in manufacturability studies. HPC enables higher throughput methods for evaluating non-equilibrium dynamics in energy storage materials.

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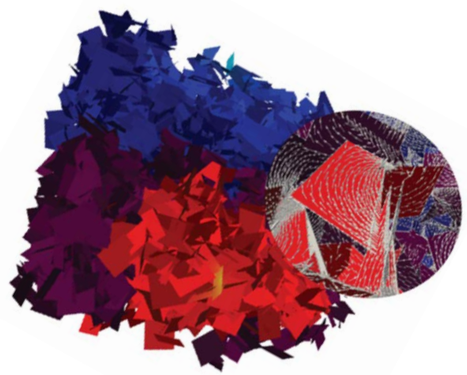
HPC Testbeds

Reservoir Labs (SBIR awardee) is one of many companies that leverage access to NERSC to improve products on their way to market. "NERSC provided Reservoir Labs with an invaluable testbed resource to prove the robustness and scalability of our R-Scope for Advanced Threat Detection product line." Large companies like Cray and other HPC vendors also leverage NERSC as the place to field test products at new scales.

Renewable Resource Modeling

The cost of drilling a geothermal well in California is roughly $5M. HPC flow simulation improves economics of geothermal over the lifetime of a field. Melior Innovations has worked with NERSC to improve the scalability of the code they use to simulate flow through geothermal fracture networks to improve reliability and economics of renewable energy. Dramatic speedups of the code have enabled new uses for simulation in geothermal. These results were published and presented at the FEniCS2015 conference.



Getting Started with NERSC

NERSC provides cutting-edge HPC resources and expertise to the Department of Energy's Office of Science research community. We specialize in reliable and advanced architectures capable of both world class simulation as well as massive data analytics. NERSC provides robust technical support to help our users get their applications running as efficiently as possible.

You can learn more about NERSC here:
www.nersc.gov

NERSC partners with programs and initiatives through allocation programs which are open to private-sector energy innovators:

- Innovative & Novel Computational Impact of Theory and Experiment (INCITE)
- ASCR Leadership Computing Challenge (ALCC)
- High Performance Computing for Manufacturing (HPC4Mfg)

Learn more here:

http://science.energy.gov/ascr/facilities/accessing-ascr-facilities/alcc
http://science.energy.gov/ascr/facilities/accessing-ascr-facilities/incite
http://www.nersc.gov/research-and-development/partnerships/
http://science.energy.gov/ascr/facilities/accessing-ascr-facilities/
https://hpc4mfg.llnl.gov/

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